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Final Report: Meta-Learning Assistants Using a Novel Characterization of Data Landscapes

#### **ABSTRACT**

Our project focused on the mathematical foundations needed to build meta-learning assistants. The overall goal is to know how we can acquire and exploit knowledge about learning (i.e., meta-knowledge) to understand and improve the performance of learning algorithms. To that end, our work focused on the following research problem: how can we decide if one single complex model, or rather a combination of simple models, is the best strategy to use when we face a supervised learning task? Our results show that a combination of simple models is often the best choice, as a minimum increase in model complexity is equivalent to tenths of simple models.

List of papers submitted or published that acknowledge ARO support during this rep	orting
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(c) Presentations
Number of Presentations: 0.00
Non Peer-Reviewed Conference Proceeding publications (other than abstracts):
Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):
Peer-Reviewed Conference Proceeding publications (other than abstracts):
(2010) Vilalta R., Ocegueda-Hernandez F., Bagaria C. A Conceptual Study of Model Selection in Classification: Multiple Local Models vs One Global Model. Second International Conference on Agents and Artificial Intelligence (ICAART-2010), Valencia, Spain.
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Number of Manuscripts: 0.00
Patents Submitted
Patents Awarded

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#### **Graduate Students**

<u>NAME</u>	PERCENT_SUPPORTED
Ricardo Vilalta	0.50
Chaitanya Bagaria	0.25
Francisco Ocegueda-Hernandez	0.25
FTE Equivalent:	1.00
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**Sub Contractors (DD882)** 

**Inventions (DD882)** 

# Final Report for Proposal No. 56268-NS-II Meta-Learning Assistants Using a Novel Characterization of Data Landscapes

Ricardo Vilalta

# **Summary of Project Activities**

Our project focused on the mathematical foundations needed to build meta-learning assistants. The overall goal is to know how we can acquire and exploit knowledge about learning (i.e., meta-knowledge) to understand and improve the performance of learning algorithms. To that end, our work focused on the following research problem: how can we decide if one single complex model, or rather a combination of simple models, is the best strategy to use when we face a supervised learning task? Our results show that a combination of simple models is often the best choice, as a minimum increase in model complexity is equivalent to tenths of simple models.

Figure 1 shows a diagram illustrating our main ideas. Traditional approaches to model selection vary complexity by jumping between model families  $F_i$ ; every single model in the new family is able to create more flexible decision boundaries compared to any single model in the first family. Alternatively, complexity can vary by combining multiple models into a composite model (while fixing the complexity of each single model in the first family); every model in the new family  $F_{ik}$  is the result of combining k models from the first family  $F_i$ . New models are also more complex but due to the composite approach. The question is how do these two approaches compare? How much complexity is precisely increased with each approach? When combining k models, how far can k increase until complexity grows above the traditional approach of invoking single complex models? By answering these questions we open the possibility of including both approaches in the same model selection strategy, while expanding our understanding of learning-algorithm designs.

#### Our Theoretical Analysis

In what follows I provide a detailed description of our theoretical analysis (a full description can be found in our conference paper at ICAART (Vilalta et al., 2010)). We showed the conditions under which combining multiple local models is expected to be beneficial. In essence we wish to compare a composite model  $M_c$  to a basic global model  $M_b$ .  $M_c$  is the combination of multiple models. We assume  $M_b$  has VC-dimension  $h_b$  and  $M_c$  has VC-dimension  $h_c$ , which comes from the combination of k models, each of VC-dimension at most k, where we assume k

The question we address is the following: how many models of VC-dimension at most h can  $M_c$  comprise to still improve on generalization accuracy over  $M_b$ , assuming both models have the same empirical error? The question refers to the maximum value of k that still gives an advantage of  $M_c$  over  $M_b$ . To proceed we look at the VC-dimension of  $h_c$ , which in essence is the VC-dimension of k-fold unions or intersections. It is an open problem to determine the VC-dimension of a family of k-fold unions (Reyzin, 2006; Blumer et al., 1989; Eisenstat and Angluin, 2007); recent work, however, shows that such a family of models has a lower bound of  $\frac{8}{5}kh$ , and an upper bound of  $2kh \log_2 3k$  (it has been shown that  $O(nk \log_2 k)$  is a tight bound (Eisenstat

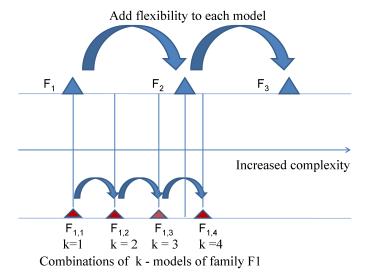


Figure 1: Two types of model selection. Top: Complexity is increased by looking at families of models  $F_i$  with increased flexibility in the decision boundaries. Bottom: Complexity is increased by combining k models while fixing the complexity of each model.  $F_{ik}$  stands for the combination of k models of family  $F_i$ . If we could compare both approaches —as in this example— we could say that model family  $F_{13}$  is less complex than family  $F_2$ , which in turn is less complex than family  $F_{14}$ .

and Angluin, 2007)). We begin our study with the lower optimistic bound, and assume the VC-dimension of  $h_c$  to be  $\frac{8}{5}kh$ . To solve the question above we equate Vapnik's guaranteed risk for both  $M_c$  and  $M_b$ :

$$\sqrt{\frac{\frac{8}{5}kh\left(\ln\frac{2N}{\frac{8}{5}kh}+1\right)-\ln(\frac{\eta}{4})}{N}} = \sqrt{\frac{h_b\left(\ln\frac{2N}{h_b}+1\right)-\ln(\frac{\eta}{4})}{N}} \tag{1}$$

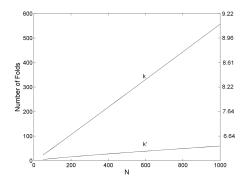
where our goal is now simply to solve for k. After some algebraic manipulation we get the following:

$$c_1k - k\ln k = c_2 \tag{2}$$

where  $c_1$  and  $c_2$  are constants:

$$c_1 = \ln 2N + 1 - \ln(\frac{8}{5}h) \tag{3}$$

$$c_2 = \frac{h_b}{\frac{8}{5}h} \left( \ln \frac{2N}{h_b} + 1 \right) \tag{4}$$



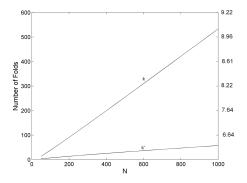


Figure 2: Left: A comparison of a compound model using k (k') support vector machines with polynomial kernels of degree one vs a simple support vector machine with a polynomial kernel of degree two; Right: same comparison except the simple support vector machine has a polynomial kernel of degree four. The degree of the polynomial kernel makes little difference in the results.

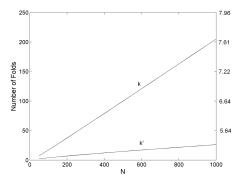
Equation 2 can be formulated as a transcendental algebraic equation. We can transform the equation as follows:

$$-c_2k^{-1}e^{-c_2k^{-1}} = -c_2e^{-c_1} (5)$$

To solve for k we can use Lambert's W function:

$$k = \frac{-c_2}{W(-c_2 e^{-c_1})} \tag{6}$$

where W can be solved using a numeric approximation.



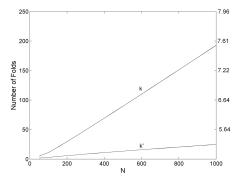


Figure 3: Left: A comparison of a compound model using k (k') support vector machines with polynomial kernels of degree two vs a simple support vector machine with a polynomial kernel of degree three; Right: same comparison except the simple support vector machine has a polynomial kernel of degree five. The degree of the polynomial kernel makes little difference in the results.

A similar analysis can be done using the upper bound of  $h_c = 2k'h \log_2 3k'$ , where we use k' to differentiate from the k used with the lower bound. After some algebraic manipulation we get the following equation:

$$c_3\nu - \nu \ln \nu = c_4 \tag{7}$$

where  $\nu = k' \ln 3k'$ , and  $c_3$  and  $c_4$  are constants (only slightly different than before):

$$c_3 = \ln 2N + 1 - \ln(\frac{2h}{\ln 2}) \tag{8}$$

$$c_4 = \frac{h_b}{\frac{2h}{\ln 2}} \left( \ln \frac{2N}{h_b} + 1 \right) \tag{9}$$

Since equations 2 and 7 have the same form,  $\nu$  has the same solution as k (equation 6):

$$\nu = \frac{-c_4}{W(-c_4 e^{-c_3})} = c_5 \tag{10}$$

We can then do the substitution back to k' to obtain the following:

$$k'\ln 3k' = c_5 \tag{11}$$

$$c_5(k')^{-1}e^{c_5(k')^{-1}} = 3c_5 (12)$$

It is now possible to solve for k':

$$k' = \frac{c_5}{W(3c_5)} \tag{13}$$

To summarize, we have shown how to express the number of k-fold (and k'-fold) unions of models, each with VC-dimension h, such that the resulting compound model exhibits the same guaranteed risk as a single model with VC-dimension  $h_b$  (we assume of course that  $h < h_b$ ). To clarify, we handle two bounds, k and k', because of our uncertainty in the VC-dimension of model unions. In principle we know there is a k'', that stands as the exact bound, below which  $M_c$  retains an advantage over  $M_b$ .

We can now study the effect on k (and k') as we vary parameters such as the size of the training set, or the VC-dimension of the models in the composite model  $M_c$  (as compared to the global model  $M_b$ ). Figures 2 and 3 show plots on how the number of model unions varies with different values of N. In each case we take the compound model as the union of k (and k') support vector machines, where the simple global model is a single support vector machine. We assume the use of polynomial kernels where the VC-dimension of each model is defined as (Burges, 1998):

$$h = \begin{pmatrix} n+p-1 \\ p \end{pmatrix} + 1 \tag{14}$$

where n is the dimensionality of the input space and p is the degree of the polynomial. In Figure 2 we assume a compound model with polynomial kernels of degree p=1. The global model varies from a polynomial degree p=2 (Figure 2-left) to a polynomial degree p=4 (Figure 2-right). In all cases we assume n=5. It is clearly observed that the value of k (k') increases linearly with N. As expected, k' corresponds to a less inclined line as the upper bound on the VC-dimension lowers the number of models we can place at the composite model while still generating less variance as the single model. In addition, a higher difference in VC-dimension (Figure 2-right) shows almost no difference in the shape of k (k') for different values of N. The right y-axis on each graph is the  $\log_2$  of the values on the left y-axis; it is simply

an indicator of how many local models we could arrange in a hierarchical structure (assuming a binary tree) while still generating less variance as the global model. We observe that for large values of N (e.g., N > 500), large hierarchies can be employed with little effect over the variance component.

Figure 3 assumes a compound model with polynomial kernels of degree p=2. The single model varies from a polynomial degree p=3 (Figure 3-left) to a polynomial degree p=5 (Figure 3-right). The same effect is observed as before except under a different scale. In all graphs we observe a large advantage gained by the combination of many low-complex models as compared to a single model exhibiting higher complexity. The difference grows linearly on N and is considerable for N>500.

#### Conclusions

Our study shows the advantage that comes when a piece-wise model fitting approach is used in classification. This is justified by the difference in the rate of complexity obtained by augmenting the number of boundaries per class (composite model) to the increase in complexity obtained by augmenting the capacity of a single global learning algorithm (classical approach). The former enables us to increase the model complexity in finer steps.

Our future goal is to use these results in building a model for the classification of classes and sub-classes in hierarchical learning problems. The key idea is to try to combine simple models as comprehensively as possible before any attempt is done to apply complex models for classification.

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